THE UNIVERSITY of EDINBURGH
informatics

Applied Machine Learning (AML)

Non-Linear Dimensionality Reduction

Oisin Mac Aodha • Siddharth N.

Outline

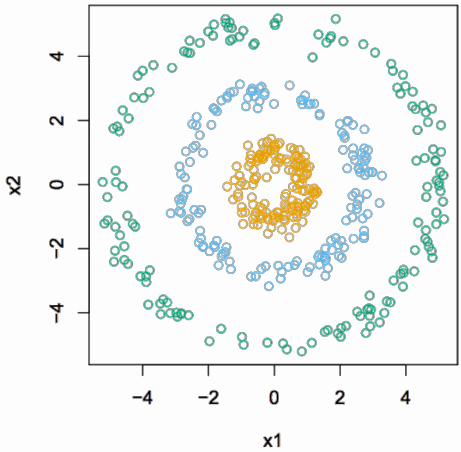
Non-Linearity

- Extensions for Linear Dimensionality Reduction
  - Kernel PCA
- Visualisation
  - Multi-Dimensional Scaling (MDS)
  - Isomap
  - Locally Linear Embeddings (LLE)
  - t-distributed Stochastic Neighbour Embedding (t-SNE)
  - Uniform Manifold Approximation & Projection (UMAP)

Extensions for Linear Dimensionality Reduction

PCA on Non-Linear Data

Example: Shells



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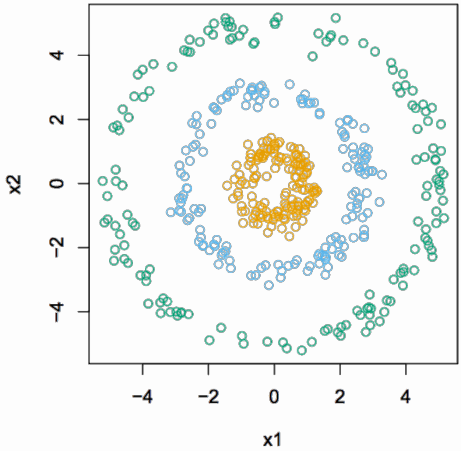

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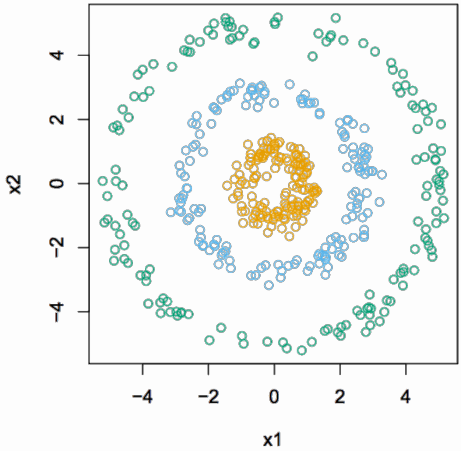

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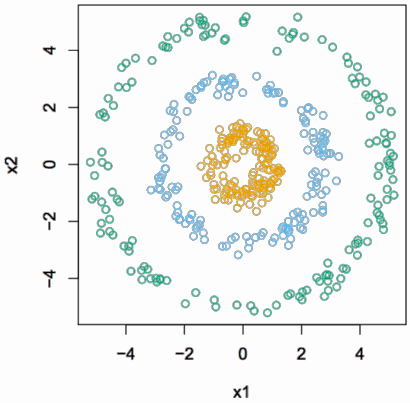

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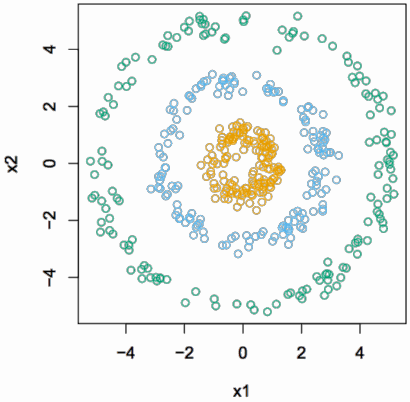

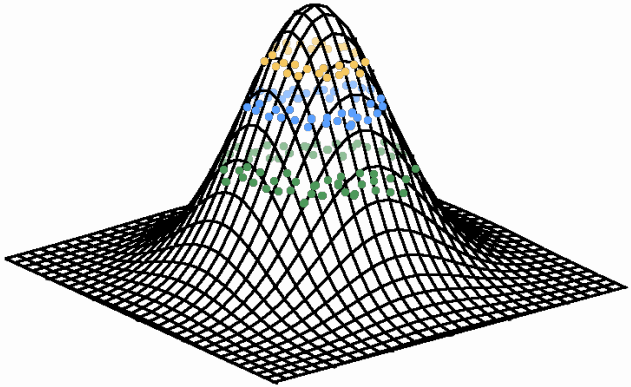

Kernel PCA

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Kernel Trick

No need to compute $\phi(\boldsymbol{x})$—only $\kappa(\boldsymbol{x}_i, \boldsymbol{x}_j)$!

Kernel PCA: Example

$$\kappa(\boldsymbol{x}_i, \boldsymbol{x}_j) = \exp\left(\frac{-\|\boldsymbol{x}_i - \boldsymbol{x}_j\|^2}{2\sigma^2}\right) \qquad \text{(RBF Kernel)}$$

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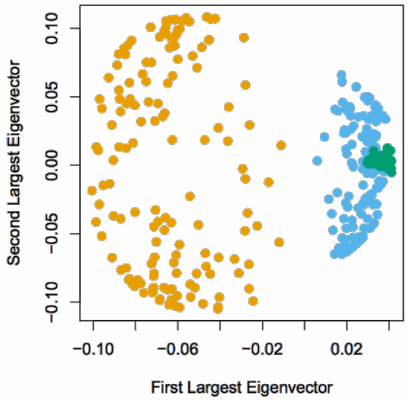
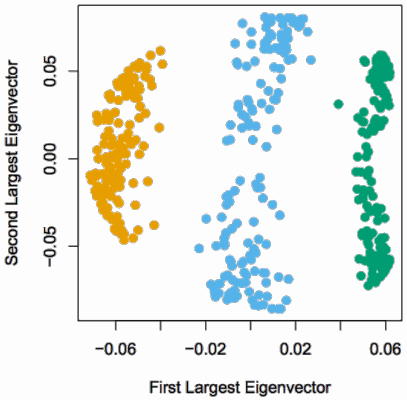


RBF ($\sigma^2 = 0.5$)



RBF ($\sigma^2 = 0.01$)

Kernel PCA

Choosing the right kernel

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Several non-linear dimensionality reduction methods can be viewed as kernel PCA, with kernels learned from data [1]

1. J. Ham et al, A Kernel View of the Dimensionality Reduction of Manifolds, 2004

Visualisation

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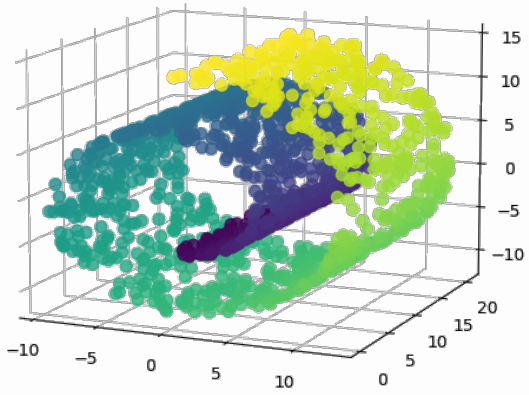

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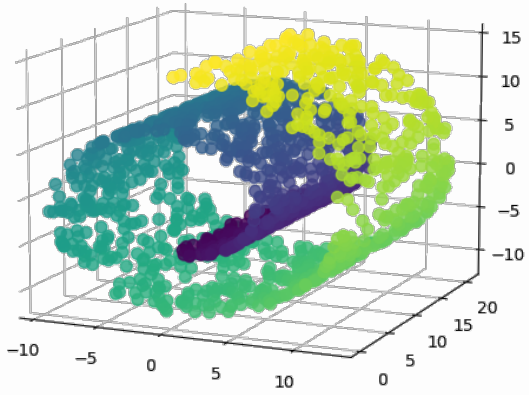

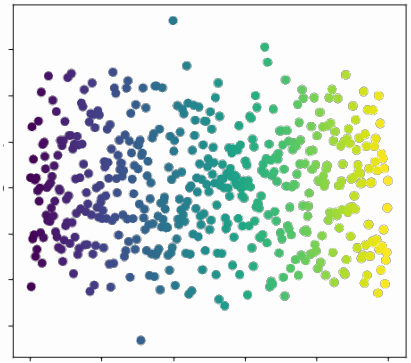

Overview

Key Ideas

- Difficult to construct a single global transformation of data
- Focus instead on some *local* measure of closeness
- Project data x onto lower-dimensional manifold as e
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- Project data $\boldsymbol{x}$ onto lower-dimensional manifold as $\boldsymbol{e}$
- **Question:** can we *preserve* local measure of closeness?

Let $\mathcal{X}$ denote the high-dimensional data space, and $\mathcal{E}$ denote the low-dimensional manifold space. We can define the following distance measures on the two spaces respectively

$$\mathcal{D}_{\mathcal{X}}(\boldsymbol{x}_i, \boldsymbol{x}_j) \qquad \mathcal{D}_{\mathcal{E}}(\boldsymbol{e}_i, \boldsymbol{e}_j)$$

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Project data from $\mathcal{X}$ to $\mathcal{E}$ while preserving the distance between *every pair of samples in original data* X

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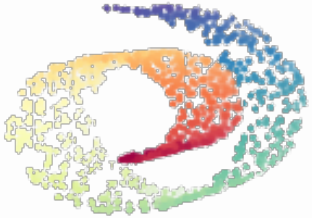
- distance metrics $\mathcal{D}_{\mathcal{X}}, \mathcal{D}_{\mathcal{E}}$ could really be anything
- choosing L_2 helps make optimisation simpler

MDS: Example

Swiss Roll



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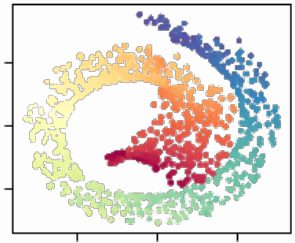

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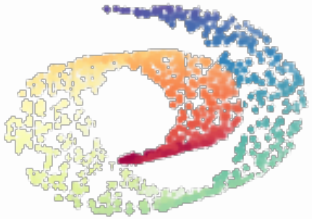

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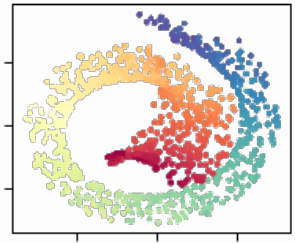

MDS (Euclidean)

- Projects down to 2D while preserving distances
- Preserving distances *outside* the manifold!

Isomap

Project data from $\mathcal{X}$ to $\mathcal{E}$ while preserving the distance between points on the *embedded manifold*, not arbitrary distance!

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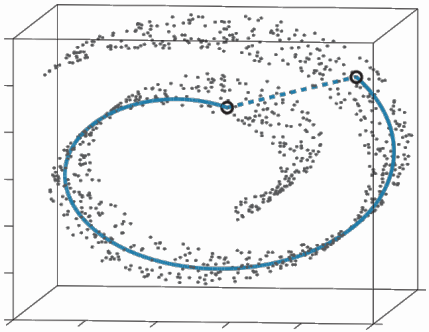

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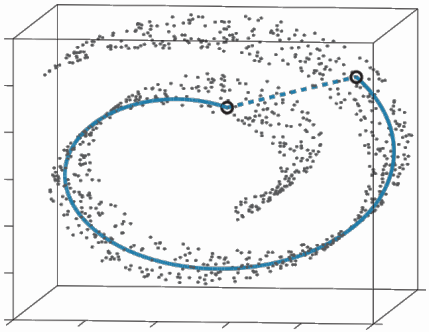

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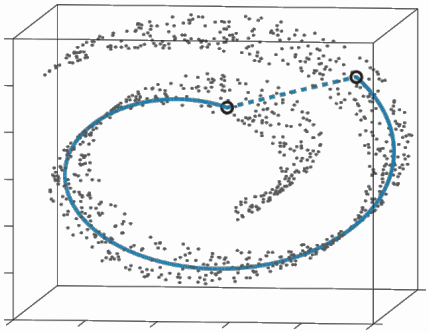

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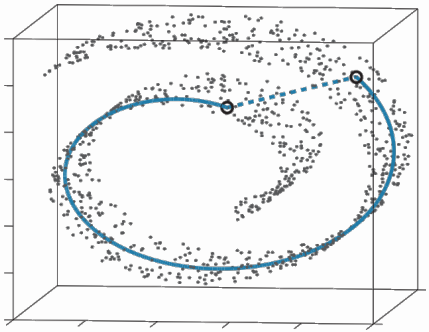

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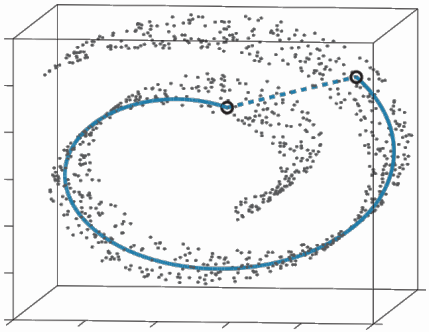

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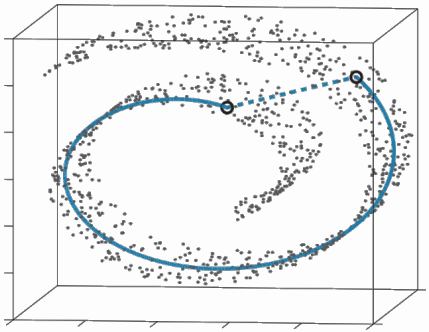

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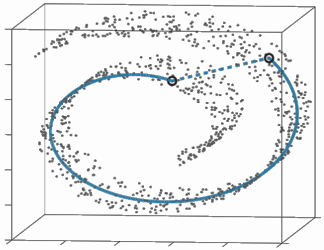
J.B. Tenenbaum et al, A Global Geometric Framework for Nonlinear Dimensionality Reduction, 2000

Isomap: Manifold



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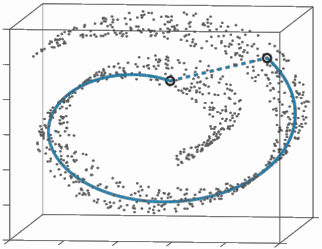

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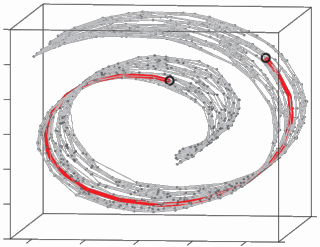

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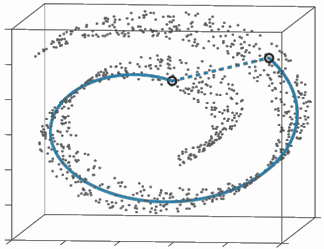

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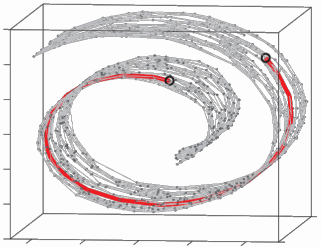

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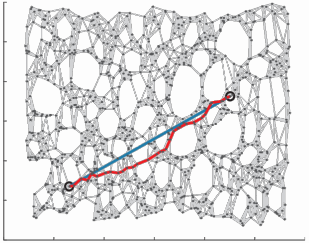

MDS

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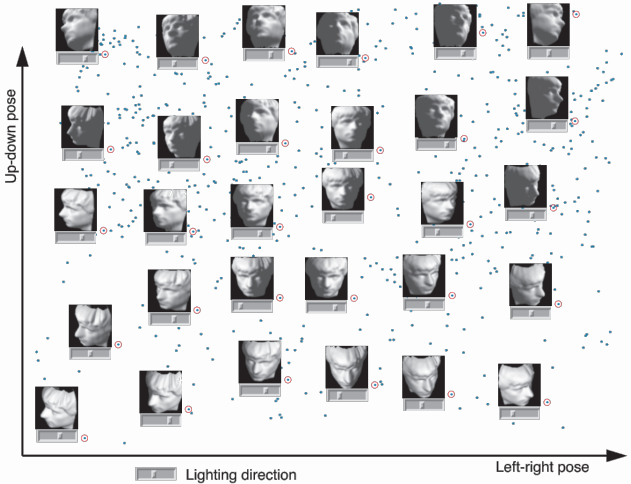

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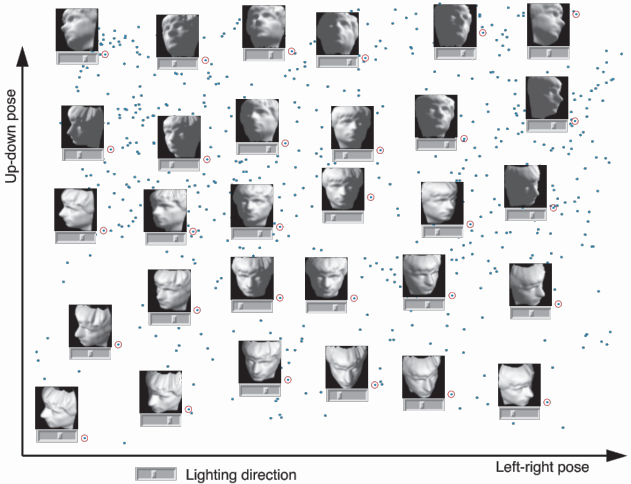

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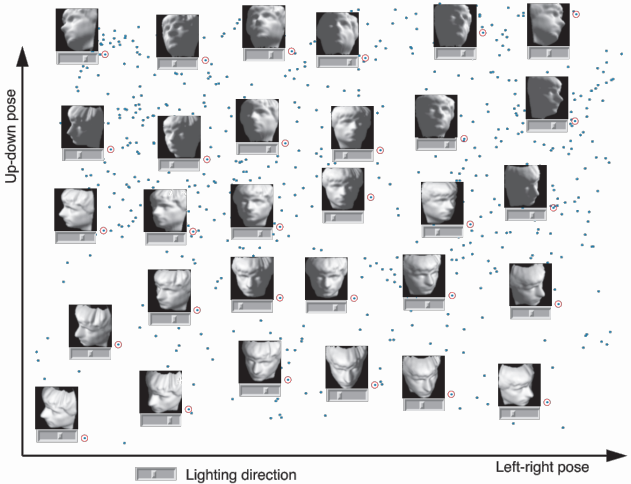

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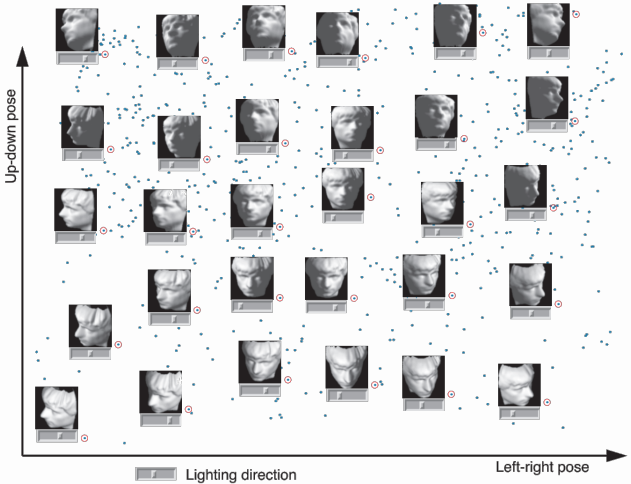

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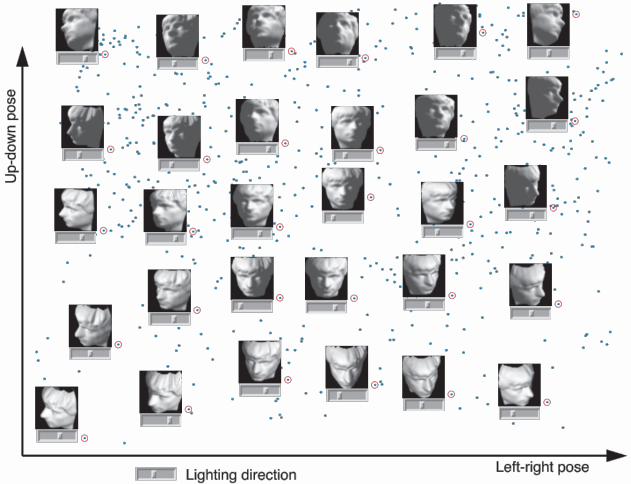

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- slow with size of data — Floyd-Warshall is $O(N^3)$!

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$$\arg\min_{w_1,\ldots,w_K} \sum_{i=1}^{N} (\boldsymbol{x}_i - \sum_{\boldsymbol{x}_k \in n(\boldsymbol{x}_i)} w_k \boldsymbol{x}_k)^2$$

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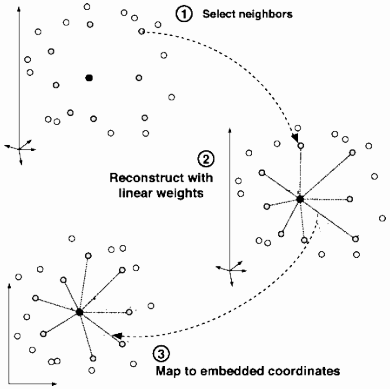

Algorithm

1. Find the weights w_k
2. Fix weights w_k and find optimal embeddings $\boldsymbol{e}_i$ solved using a (sparse) eigen-decomposition

Locally Linear Embeddings (LLE)

Project data from $\mathcal{X}$ to $\mathcal{E}$ while preserving the *linear transform that reconstructs points* from the K nearest neighbours

$$\arg\min_{w_1,\ldots,w_K} \sum_{i=1}^{N} (\boldsymbol{x}_i - \sum_{\boldsymbol{x}_k \in n(\boldsymbol{x}_i)} w_k \boldsymbol{x}_k)^2$$

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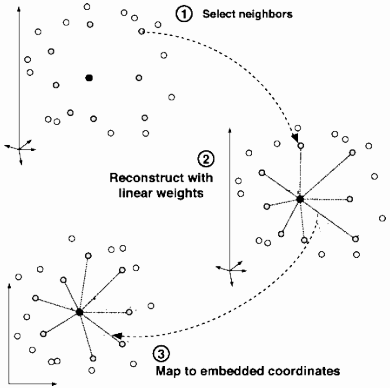

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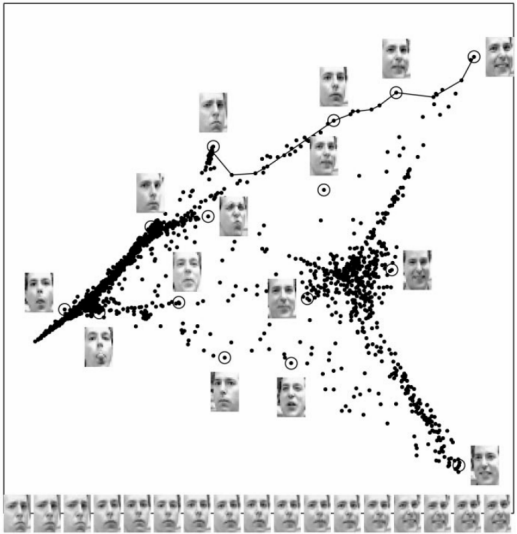
S.T. Roweis & L.K. Saul, Nonlinear dimensionality reduction by locally linear embedding, 2000

LLE: Example and Issues



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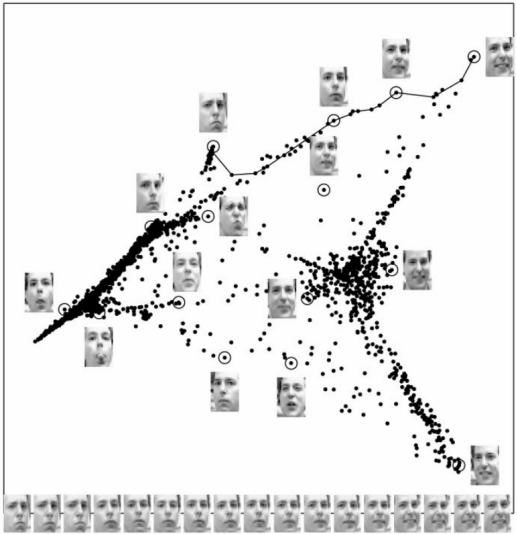

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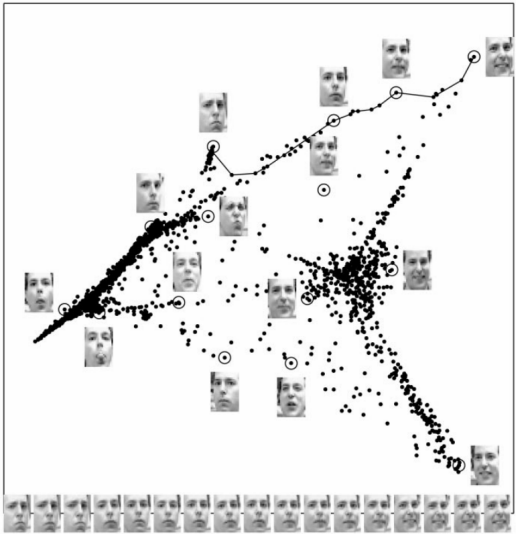

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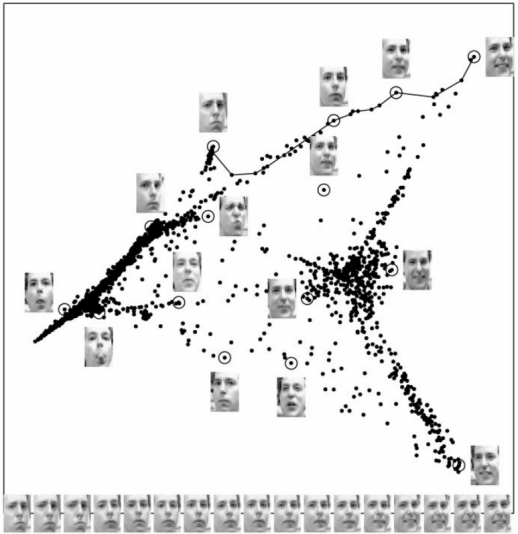

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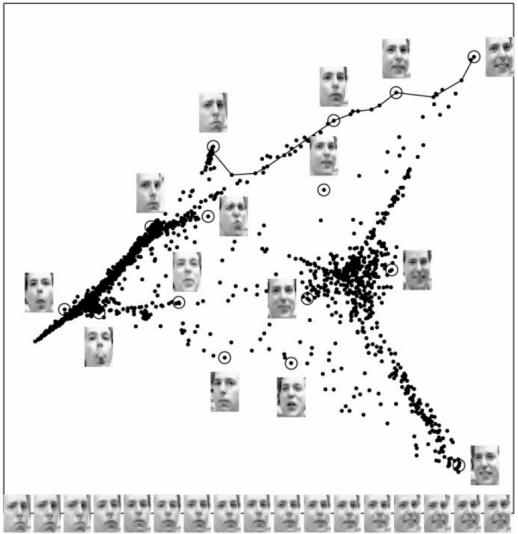

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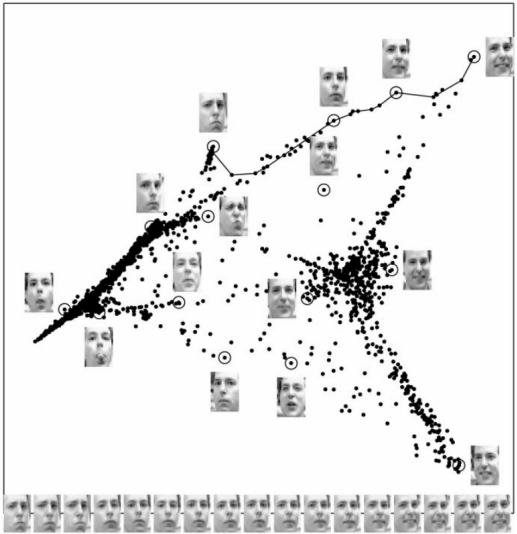

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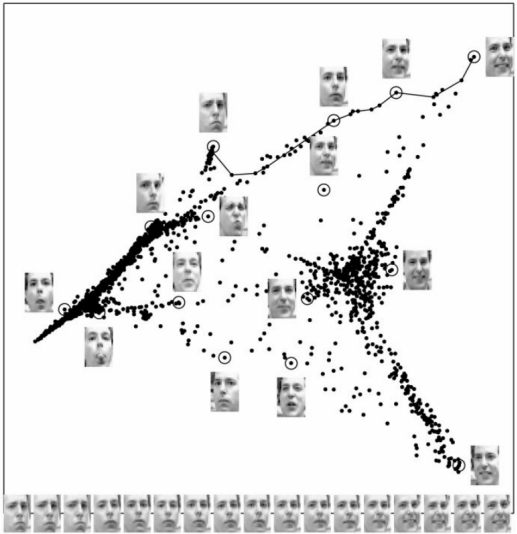

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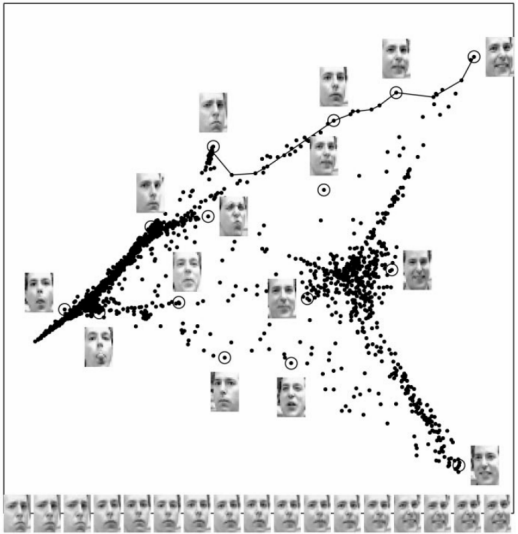

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Project data from $\mathcal{X}$ to $\mathcal{E}$ while preserving the *probability distribution over pairwise similarities* between points in the space.

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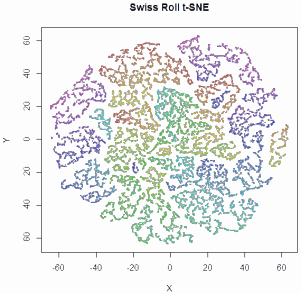
Objective: $\min \mathrm{KL}\big(\mathcal{D}_{\mathcal{X}}(\boldsymbol{x}_i, \boldsymbol{x}_j) \| \, \mathcal{D}_{\mathcal{E}}(\boldsymbol{e}_i, \boldsymbol{e}_j)\big)$

L.J.P. van der Maaten & G.E. Hinton, Visualizing Data using t-SNE, 2008

t-SNE: Examples



Figures: https://jlmelville.github.io/uwot/umap-examples.html

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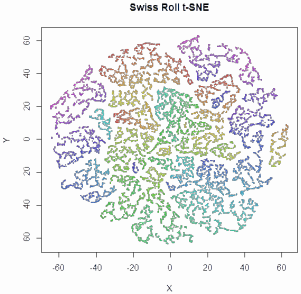

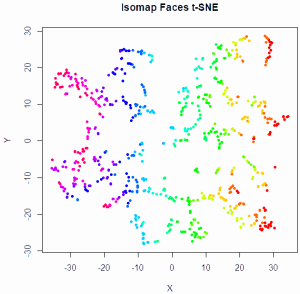

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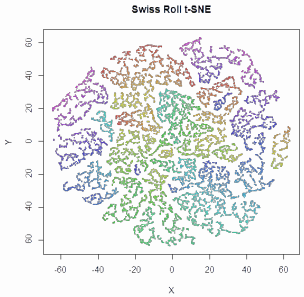

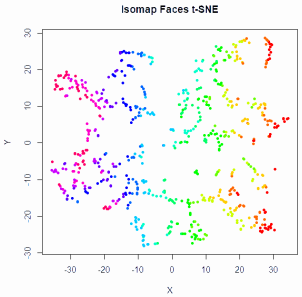

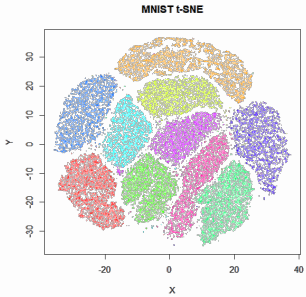

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Issue

None of these methods learn an *explicit* metric

- $\{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\} \xrightarrow{f} \{\boldsymbol{e}_1, \ldots, \boldsymbol{e}_N\}$ but $\boldsymbol{x}_t \xrightarrow{\not{f}} \boldsymbol{e}_t$ for unseen $\boldsymbol{x}_t$
- cannot project an unseen point without redoing the optimisation!

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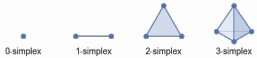

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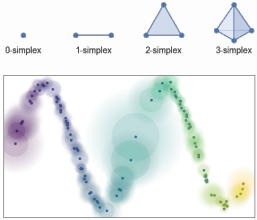

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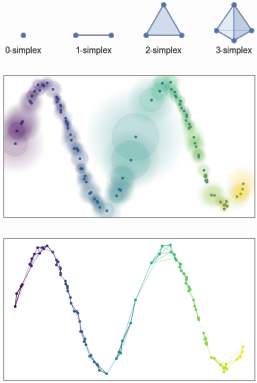
Overview

- Use simplices as basic building block
- Estimate connectivity and distances between points
- Construct graph that captures topology of manifold!



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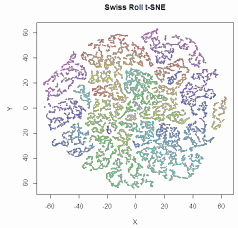
Advantages

- Can learn a metric, so computing $\boldsymbol{x}_t \xrightarrow{f} \boldsymbol{e}_t$ for unseen $\boldsymbol{x}_t$ is feasible (when labels available)!
- Is fast and scalable
- Can be run unsupervised, supervised, or even weakly supervised!

UMAP: Examples and Comparisons

t-SNE



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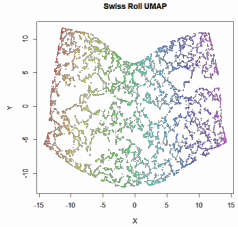

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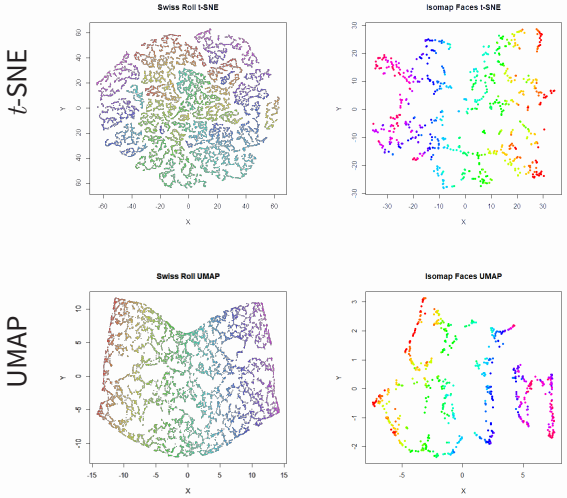

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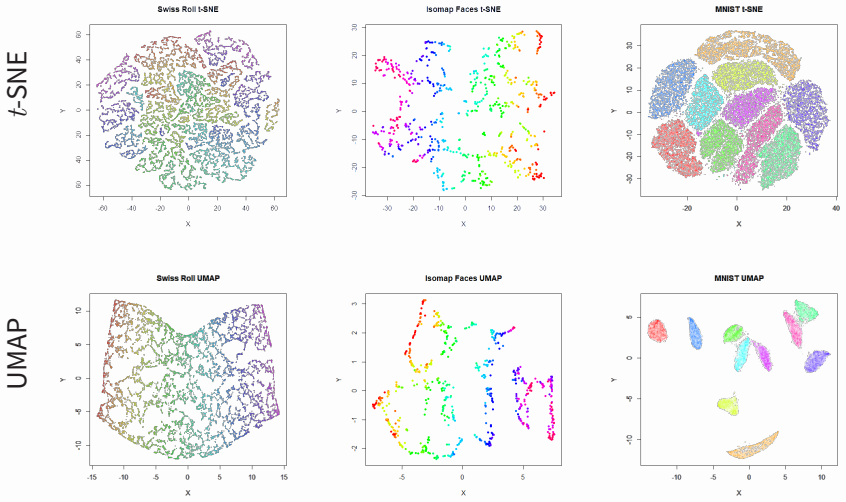

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- Many approaches to choose from—t-SNE and UMAP most popular